2-hydroxy-3-methyl-2-(propan-2-yl)butanoic acid
5438-17-5 | DTXSID50280375

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 238 °C

Global applicability domain: Inside

Local applicability domain index: 2.74e-01

Confidence level: 3.39e-01

Nearest Neighbors from the Training Set

Image not found
2-Hydroxyisobutyric acid
Measured: 212
Predicted: 214

Image not found
2-Hydroxyphenylacetic acid
Measured: 240
Predicted: 261

Image not found
Chloral hydrate
Measured: 98.0
Predicted: 123

Image not found
1-Methylcyclohexanecarboxylic acid
Measured: 234
Predicted: 239